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EFFECTIVE POTENTIAL OF ELECTRON-ELECTRON INTERACTION IN THE SEMIINFINITE ELECTRON GAS WITH REGARD FOR THE LOCAL-FIELD CORRECTION

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The effective potential of electron–electron interaction and the two-particle "density–density" correlation function have been calculated for a simple semiinfinite metal making allowance for the local-field correction. The influences of a flat interface and various models of local-field correction on the results of calculations are analyzed.

K e y w o r d s: semiinfinite metal, jellium model, effective potential, correlation function.

1. Introduction

The modern quantum-mechanical statistical theory of Fermi systems with an interface is still far from being completed. The urgency in the theoretical description of such systems can hardly be overestimated owing to the importance of processes that occur in the presence of an interface and a rapid development of experimental methods aimed at surface researches.

The most popular theoretical method to study such systems is the density functional one [1], which was created on the basis of the well-known Thomas–Fermi approximation firstly developed for atoms. By its nature, the density functional method is a one-particle approach, so it cannot consider many-body correlation effects correctly. Therefore, the energy functionals of systems with an interface are most often considered in the local density approximation; namely, the expressions known from the theory of uniform systems are taken for calculations, but the distribution of the electron density $n(\mathbf{r})$ is substituted for the electron concentration n. This approach is debatable [2], because the interface introduces not only quantitative, but also qualitative changes in various parameters of the electron system (e.g., the image forces emerge and so on), which cannot be taken into account in principle by the density functional theory.

In the cycle of works [3–9], an attempt was made to develop a consistent quantum-mechanical statistical theory for a simple metal with the interface "metal–vacuum". In particular, it was shown that the thermodynamic potential and the structural distribution functions of electrons in a semiinfinite metal are expressed in terms of the effective electron-electron interaction potential. This work logically continues this cycle of works. It was aimed at studying the influence of various approximations for the local-field correction on the two-particle correlation function "density–density" and the effective potential of electron-electron interaction.

The effective interaction between charged particles in spatially confined systems attracts the attention of researchers for a long time. In particular, it was studied in works [10–18]. In work [10], under certain approximations, the polarization part of the energy of interaction between a motionless point charge and a semiinfinite metal was calculated. Using similar approximations, the dielectric function of a semiinfinite metal and the effective potential were calculated in work [11]. In works [12, 13] in the framework of

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the effective interaction potential approximation, the asymptotics of Friedel oscillations at large distances between charges at the interface was obtained, and their dependence on the Fermi surface shape in metals were studied.

In works [14–17], the screening of a charged impurity near the metal surface was studied in the random-phase approximation. In particular, the dependences of the electrostatic potential of this impurity on the distance in the surface plane and the distance to the surface were calculated in the quasiclassical case and the Thomas–Fermi approximation, and Friedel oscillations were revealed.

In order to eliminate shortcomings inherent to the density functional method, attempts were made to use the GW approach [19] with the density functional method. In particular, in work [18], the effective potential of electron-electron interaction was calculated with the use of the local density approximation for the exchange-correlation potential.

2. Model

Consider a semiinfinite simple metal in the framework of the jellium model, i.e. when the ionic subsystem of a metal is represented by a uniformly distributed positive charge confined by the interface plane $z = -d$, with the density

$$n_+(x,y,z) \equiv n_+(z) = n_{\text{bulk}}\,\theta(-d-z), \tag{1}$$

where

$$\theta(x) = \begin{cases} 1, & x > 0, \\ 0, & x < 0 \end{cases}$$

is the Heaviside function, n_{bulk} is the electron concentration, and $d > 0$ is a parameter determined self-consistently from the electroneutrality condition

$$\int\limits_{-\infty}^{+\infty} \mathrm{d}z\,(n(z) - n_+(z)) = 0, \tag{2}$$

where $n(z)$ is the electron density distribution. Let the ionic subsystem form a surface potential for electrons in the metal, which does not allow them to escape. This surface potential is simulated by the potential wall

$$V(z) = \begin{cases} \infty, & z \geqslant 0, \\ 0, & z < 0. \end{cases} \tag{3}$$

This model of potential physically correctly corresponds to a real situation and allows analytical solutions to be obtained for the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\Delta + V(z)\right]\Psi_{\mathbf{p},\alpha}(\mathbf{r}) = E_\alpha(\mathbf{p})\Psi_{\mathbf{p},\alpha}(\mathbf{r}),$$

where m is the electron mass, $\hbar\mathbf{p}$ the two-dimensional vector of electron momentum in the plane parallel to the interface, and α the quantum number associated with the electron motion normally to the interface. Since the electron moves freely in parallel to the interface, the wave function and the corresponding energy of the electron can be written as follows:

$$\Psi_{\mathbf{p},\alpha}(\mathbf{r}) = \frac{1}{\sqrt{S}}\mathrm{e}^{\mathrm{i}\mathbf{p}\mathbf{r}_{||}}\varphi_\alpha(z), \quad E_\alpha(\mathbf{p}) = \frac{\hbar^2(p^2+\alpha^2)}{2m}.$$

Here, $\mathbf{r} = (\mathbf{r}_{||}, z)$ is the radius vector of the electron, S is the interface area, and

$$\varphi_\alpha(z) = \frac{2}{\sqrt{L}}\sin(\alpha z)\theta(-z),\ \alpha = \frac{2\pi n}{L},\ n = 1,2,...,$$

where L determines the variation range of the electron coordinate normal to the interface: $z \in \in [-L/2, +\infty)$. The parameters L and S tend to infinity, so that the problem is considered in the thermodynamic limit.

3. Effective Potential of Electron-Electron Interaction

According to work [6], the two-dimensional Fourier transform of the effective potential of electron-electron interaction with respect to the radius vector $\mathbf{r}_{||}$ can be expressed in the form

$$g(q|z_1,z_2) = \nu(q|z_1-z_2) + \\ + \frac{\beta}{SL^2}\int\limits_{-L/2}^{+\infty}\mathrm{d}z\int\limits_{-L/2}^{+\infty}\mathrm{d}z'\nu(q|z_1-z)\times \\ \times\mathfrak{M}(q|z,z')\nu(q|z'-z_2), \tag{4}$$

where

$$\nu(q|z_1-z_2) = \frac{2\pi e^2}{q}\,\mathrm{e}^{-q|z_1-z_2|}$$

is the two-dimensional Fourier transform of the Coulomb potential, z_1 and z_2 are the coordinates of electrons reckoned normally to the interface, β the inverse thermodynamic temperature, and $\mathfrak{M}(q|z,z')$

the "density–density" correlation function, which is a solution of the Fredholm integral equation of the second kind [7],

$$\mathfrak{M}(q|z_1,z_2)=\mathfrak{M}_0(q|z_1,z_2)+$$
$$+\frac{\beta}{SL^2}\int\limits_{-L/2}^{+\infty}\mathrm{d}z\int\limits_{-L/2}^{+\infty}\mathrm{d}z'\mathfrak{M}_0(q|z_1,z)\times$$
$$\times\Big(\nu(q|z-z')-\overline{\nu}(q|z-z')\Big)\mathfrak{M}(q|z',z_2), \qquad (5)$$

where $\overline{\nu}_k(q)=G_k(q)\nu_k(q)$, $\nu_k(q)=\frac{4\pi e^2}{q^2+k^2}$ is the three-dimensional Fourier transform of the Coulomb potential (the variable k is responsible for the Fourier expansion along the electron coordinate normal to the interface),

$$\overline{\nu}(q|z-z')=\frac{1}{L}\sum_k \mathrm{e}^{\mathrm{i}k(z-z')}\overline{\nu}_k(q),$$

$\mathfrak{M}_0(q|z_1,z_2)$ is the two-particle "density–density" correlation function in the ideal exchange approximation [7], and $G_k(q)$ is the local-field correction.

In the low-temperature limit, the following expression was obtained in work [6] for the two-particle correlation function of an electron gas in the ideal exchange approximation:

$$\mathfrak{M}_0(q|z_1,z_2)=\frac{L^2}{\beta}\sum_{\alpha_1,\alpha_2}\Lambda_{\alpha_1,\alpha_2}(q)\times$$
$$\times\varphi^*_{\alpha_1}(z_1)\varphi_{\alpha_2}(z_1)\varphi^*_{\alpha_2}(z_2)\varphi_{\alpha_1}(z_2), \qquad (6)$$

where

$$\Lambda_{\alpha_1,\alpha_2}(q)=\frac{2m}{\hbar^2}\frac{S}{2\pi}\frac{\alpha_1^2-\alpha_2^2-q^2}{q^2}\times$$
$$\times\left[1-\sqrt{1-4q^2\frac{p_{\mathrm{F}}^2-\alpha_1^2}{(\alpha_1^2-\alpha_2^2-q^2)^2}}\times\right.$$
$$\left.\times\,\theta\left(1-4q^2\frac{p_{\mathrm{F}}^2-\alpha_1^2}{(\alpha_1^2-\alpha_2^2-q^2)^2}\right)\right]\theta(p_{\mathrm{F}}-\alpha_1), \qquad (7)$$

$p_{\mathrm{F}}=(9\pi/4)^{1/3}/r_{\mathrm{S}}$ is the Fermi momentum, and r_{S} the Brueckner parameter in the units of the Bohr radius a_{B}.

In work [6], it was shown that, in some approximations, an analytical expression can be obtained for the function $\mathfrak{M}_0(q|z_1,z_2)$,

$$\mathfrak{M}_0(q|z,z')=-\frac{SL^2}{\beta}\frac{2m}{\hbar^2}\frac{1}{\pi^2}\frac{\mathrm{e}^{-q|z-z'|}-\mathrm{e}^{-q|z+z'|}}{q}\times$$
$$\times\left[\frac{p_{\mathrm{F}}\cos(p_{\mathrm{F}}(z+z'))}{(z+z')^2}-\frac{p_{\mathrm{F}}\cos(p_{\mathrm{F}}(z-z'))}{(z-z')^2}+\right.$$
$$\left.+\frac{\sin(p_{\mathrm{F}}(z-z'))}{(z-z')^3}-\frac{\sin(p_{\mathrm{F}}(z+z'))}{(z+z')^3}\right]\times$$
$$\times\,\theta(-z)\theta(-z'). \qquad (8)$$

From this expression, one can see, in particular, that, besides the terms, which depend on $(z-z')$ and are characteristic of uniform systems, there are terms depending on $(z+z')$. The reason for their appearance is the presence of the plane interface. This means that, in our ideal-exchange approximation for the two-particle "density–density" correlation function, the image-force effects are already taken into consideration. Note that the polarization operator in works [10, 11] is presented as a sum of two polarization operators for the uniform electron gas: one of them depends on $(z-z')$, and the other on $(z-z')$. However, formula (8) shows that the dependences of $\mathfrak{M}_0(q|z_1,z_2)$ on $(z-z')$ and $(z+z')$ are not so simple.

In the following numerical calculations of the two-particle "density–density" correlation function in the ideal exchange approximation, expression (6) is used.

4. Results of Numerical Calculations of Two-Particle "Density–Density" Correlation Function and Effective Electron-Electron Interaction Potential

The two-particle "density–density" correlation function of electrons, $\mathfrak{M}(q|z_1,z_2)$, was numerically calculated according to Eq. (5) and making allowance for the local-field correction $G_k(q)$ taken from the theory of uniform electron gas in the following forms:

1) the modified Hubbard correction [20]

$$G_k(q)=\frac{1}{2}\frac{q^2+k^2}{q^2+k^2+\xi p_{\mathrm{F}}^2}, \qquad (9)$$

where ξ is a parameter, the values of which are given below; and

2) the Ichimaru correction [21]

$$G_k(q)=AQ^4+BQ^2+C+$$
$$+\left[AQ^4+\left(B+\frac{8}{3}A\right)Q^2-C\right]\times$$
$$\times\frac{4-Q^2}{4Q}\ln\left|\frac{2+Q}{2-Q}\right|, \qquad (10)$$

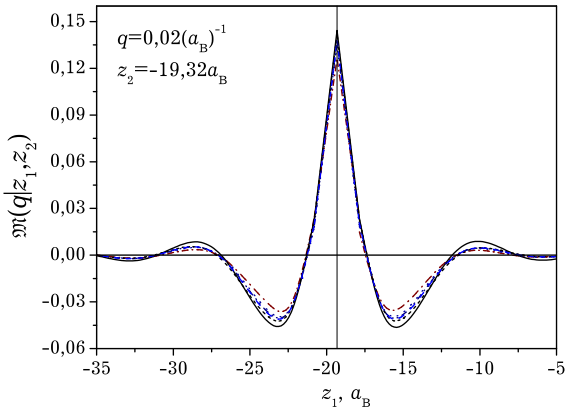

Fig. 1. Dependences of the dimensionless two-particle "density–density" correlation function on the coordinate of electron 1 normal to the interface, whereas the corresponding coordinate of electron 2 is fixed ($z_1 = -19.57a_{\rm B}$); $q = 0.02a_{\rm B}^{-1}$

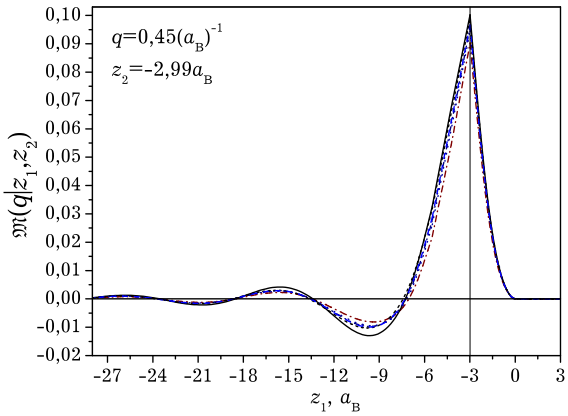

Fig. 2. The same as in Fig. 1, but for $z_1 = -2.99a_{\rm B}$ and $q = 0.45a_{\rm B}^{-1}$

Table 1. **Legends of the figures**

Line type	Approximation
———	Animalu
– – – –	Geldart and Vosko ($\xi = 2$)
– · – · –	$G_k(q) \equiv 0$
– – – – –	Hubbard ($\xi = 1$)
·····	Sham ($\xi = 1 + \frac{4}{\pi p_{\rm F} a_{\rm B}}$)
– · – · – ·	Animalu ($\xi = 1 + \frac{2}{\pi p_{\rm F} a_{\rm B}}$)

where $Q = \sqrt{q^2 + k^2}/p_{\rm F}$, and the parameters A, B, and C are cumbersome and can be found in work [21].

All numerical calculations were carried out for potassium ($r_{\rm S} = 4.86\, a_{\rm B}$).

Substituting the numerical solution of Eq. (5) into formula (4), we obtain a two-dimensional Fourier transform of the effective potential of electron-electron interaction. Making the inverse Fourier transformation with respect to the variable $\mathbf{q}$ and taking into account that the two-dimensional Fourier transform of the effective potential depends only on the absolute value of the vector $\mathbf{q}$, we obtain the effective potential of electron-electron interaction in the form

$$g(r_\parallel, z_1, z_2) = \frac{1}{S}\sum_{\mathbf{q}} {\rm e}^{{\rm i}\mathbf{q}\mathbf{r}_\parallel} g(q|z_1, z_2) =$$
$$= \frac{1}{2\pi}\int\limits_0^\infty {\rm d}q\, q\, {\rm J}_0(qr_\parallel) g(q|z_1, z_2),$$

where ${\rm J}_0(x)$ is the zeroth-order cylindrical Bessel function.

In Figs. 1 to 3, the results of calculations of the two-particle "density–density" correlation function of electrons, $\mathfrak{M}(q|z_1, z_2)$, obtained by solving the Fredholm integral equation of the second kind (5) making allowance for various local-field corrections and without them (the random-phase approximation) are depicted. If one of the electrons is in the metal depth, this function is symmetric with respect to the coordinate of a fixed electron directed normally to the interface plane and has a sharp peak, when those coordinates of two electrons coincide (see Fig. 1), i.e. the electrons correlate with each other and do not feel the influence of the surface. If one of the electrons approaches the interface, the latter starts to affect the two-particle correlation function of electrons. The sharp symmetric peak that was observed in Fig. 1 loses its symmetry and broadens: besides electron correlations, there emerges an effective repulsion from the interface (see Fig. 2). This repulsion results in the following. When the electron approaches the interface even more, the maximum in the two-particle correlation function of electrons does not occurs, when their coordinates coincide, as it was in the metal depth (see Fig. 1), but is a little shifted to the left from the interface (in Fig. 3, this maximum is located at about $-2.7a_{\rm B}$).

In addition, Figs. 1 to 3 demonstrate that various models of the local-field correction do not change the behavior of the two-particle correlation function of electrons qualitatively, but do it quantitatively. The application of the random-phase approximation produces the smallest deviations in the two-particle correlation function of electrons, whereas the Ichimaru

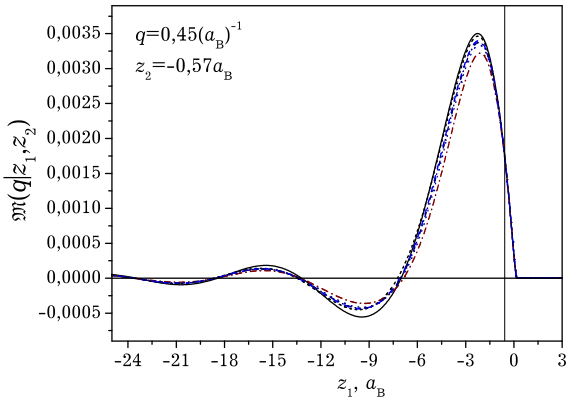

Fig. 3. The same as in Fig. 1, but for $z_1 = -0.57a_B$ and $q = 0.45a_B^{-1}$

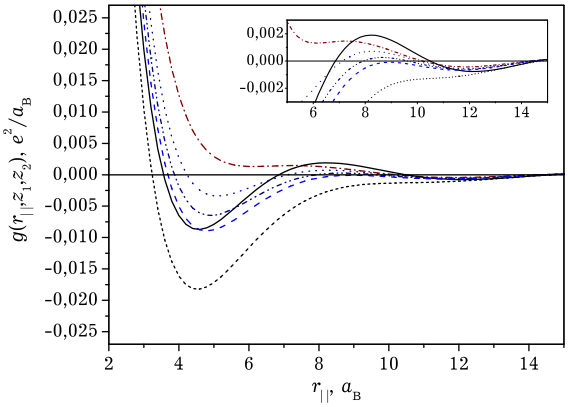

Fig. 4. Dependences of the effective electron-electron interaction potential on the distance between the electrons along the interface. The electron coordinates $z_1$and z_2 normal to the interface are identical and fixed. The case $(z_1, z_2) \to -\infty$. The notation of curves is the same as in Fig. 1

correction leads to the largest ones. The calculated values of two-particle correlation function for electrons with the use of other local-field corrections fall within the interval between the values obtained in the random-phase approximation and with the use of the Ichimaru correction.

In Fig. 4 to 9, the results of calculations for the effective potential of electron-electron interaction $g(r_\parallel, z_1, z_2)$ obtained for various local-field correction models and without them (the random-phase approximation) are shown. In Fig. 4, the effective potential of interaction between electrons located in the metal depth, i.e. when they do not feel the interface influence, is exhibited. From this figure, one can see that making allowance for the local-field correction brings about the appearance of a potential well at distances from 4.5 to 5 times a_B, depending on the specific correction model. The depth of this potential well also depends on the local-field correction

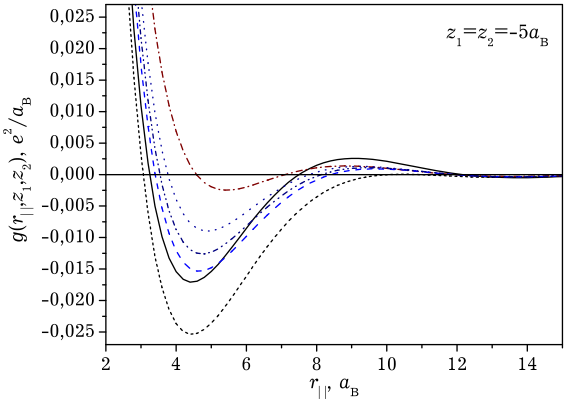

Fig. 5. The same as in Fig. 4, but for $z_1 = z_2 = -5a_B$

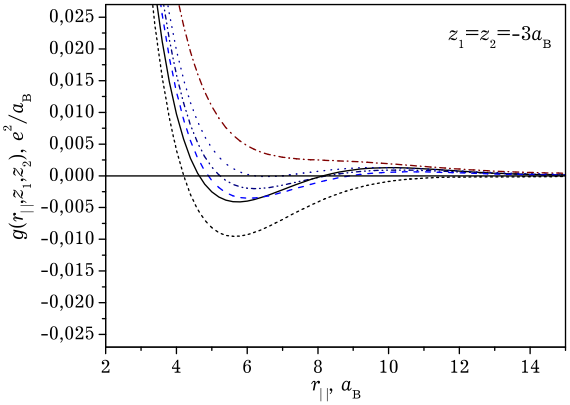

Fig. 6. The same as in Fig. 4, but for $z_1 = z_2 = -3a_B$

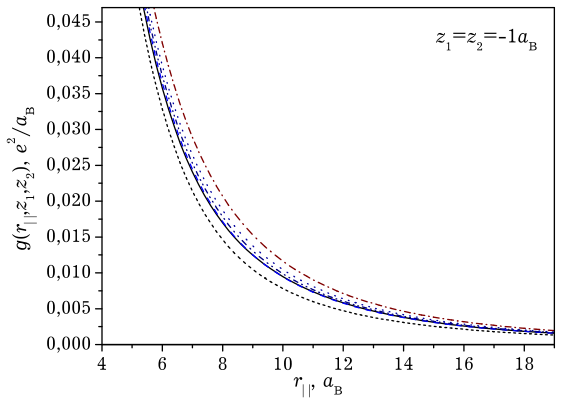

Fig. 7. The same as in Fig. 4, but for $z_1 = z_2 = -a_B$

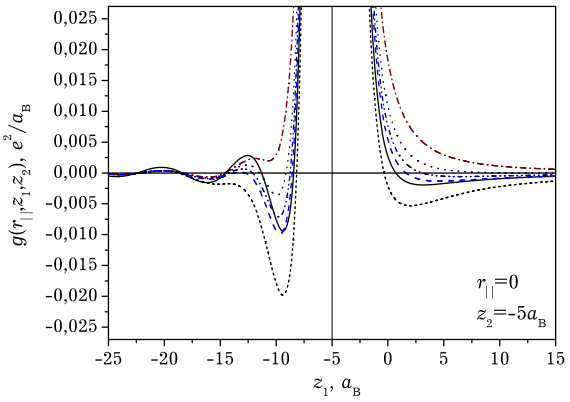

Fig. 8. Dependences of the effective electron-electron interaction potential on the distance from electron 1 to the interface. The normal coordinate of electron 2 is fixed, $z_2 = -5a_{\rm B}$, $r_{\parallel} = = 0$. The notation of curves is the same as in Fig. 1

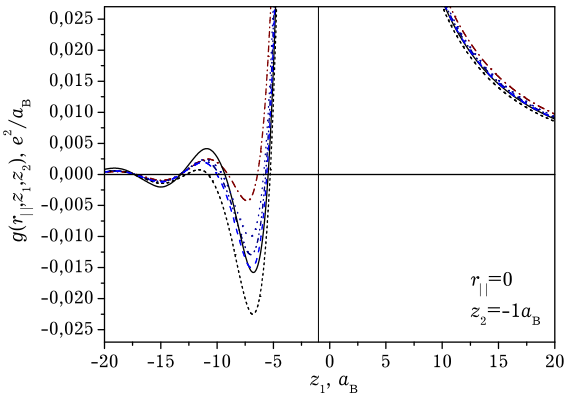

Fig. 9. The same as in Fig. 8, but for $z_2 = -a_{\rm B}$

model. The deepest potential well corresponds to the Hubbard correction, and the shallowest one to the Sham model. Other examined corrections give rise to intermediate depths of the potential well. In addition, in the random-phase approximation (i.e. when the local-field correction is not taken into consideration, the dash-dotted curve), there is no potential well at indicated distances in the case of a uniform system. At large distances, there emerge Friedel oscillations [12,13,22]. However, in the case of the effective potential calculated in work [18], they are absent.

In Fig. 5, the dependence of the effective electron-electron interaction potential on the distance between the electrons is depicted for the normal coordinates of electrons $z_1 = z_2 = -5a_{\rm B}$. For this distance of electrons from the interface, a considerable deepening of the potential well is observed; moreover, it appears even in the random-phase approximation. This fact originates from a nonmonotonic behavior of the electron density distribution $n(z)$ near the interface [4]; namely, here, the plane layers with electron concentrations lower and higher than that in the metal depth alternate. As a result, the collective effects in the electron-enriched layers are more pronounced, and the electron screening is stronger. In the electron-depleted layers, the situation is opposite: the screening is weaker, and the repulsion between electrons becomes stronger (see Fig. 6). If the electrons come nearer to the interface, the repulsion between them prevails (Fig. 7). As the coordinates of electrons normal to the interface grow further, the effective potential of electron-electron interaction tends to the Coulomb potential:

$$\lim_{z_1,z_2\to\infty} g(r_{\parallel},z_1,z_2) = \frac{e^2}{\sqrt{r_{\parallel}^2+(z_1-z_2)^2}}.$$

The same behavior is demonstrated in Figs. 8 and 9. They exhibit the dependence of the effective potential of interaction between the electrons located on the same normal to the interface ($r_{\parallel} = 0$) on the normal coordinate of one of the electrons, regarding the other electron to be fixed. The presence of the interface results in a nonsymmetric effective potential of electron-electron interaction with respect to the electron coordinate normal to the interface. There are more electrons to the left from the fixed one, and the screening is stronger; therefore, the potential wells and Friedel oscillations are observed; to the right, the number of electrons is smaller, so that the potential well is either shallower or disappears.

5. Conclusions

To summarize, the two-particle correlation function of electrons and the effective potential of electron-electron interaction have been calculated making allowance for various local-field correction models known in the theory of uniform electron gas. The behavior of the two-particle correlation function of electrons depending on the electron coordinates normal to the interface is studied, as well as the influence of various local-field correction models on it. In particular, it is found that the presence of the interface gives rise to an additional effective repulsion of the electrons from the interface, the maximum of the

two-particle correlation function does not take place at the coincidence of electron coordinates, as occurs in the metal depth, but is a little shifted from the interface.

The behavior of the effective electron-electron interaction potential depending on the electron coordinates normal to the interface and the distance between the electrons along the interface is also examined, as well as the influence of various local-field correction models on it. The results of our calculations demonstrate that, in the near-surface region of the metal, there are plane layers, where the behavior of the effective potential of electron-electron interaction is essentially different. Namely, in some layers, the effective potential oscillates and form deep potential wells, whereas the wells are shallower or even absent in other layers. As a result, the additional mechanical stresses emerge near the metal surface, which can provoke the appearance of cracks and other defects.

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ЕФЕКТИВНИЙ ПОТЕНЦІАЛ
МІЖЕЛЕКТРОННОЇ ВЗАЄМОДІЇ
ДЛЯ НАПІВОБМЕЖЕНОГО ЕЛЕКТРОННОГО ГАЗУ
З ВРАХУВАННЯМ ПОПРАВКИ НА ЛОКАЛЬНЕ ПОЛЕ

Р е з ю м е

У роботі проведено чисельний розрахунок ефективного потенціалу міжелектронної взаємодії та двочастинкової кореляційної функції електронів "густина–густина" для напівобмеженого простого металу з урахуванням поправки на локальне поле. Досліджено вплив на них плоскої поверхні поділу та різних форм поправки на локальне поле. Показано, що біля поверхні поділу є області з більшою глибиною потенціальної ями у ефективному потенціалі міжелектронної взаємодії, ніж в глибині металу.